

Succinic acid, 2-naphthylmethyl 2-octyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C23H30O4/c1-3-4-5-6-9-18(2)27-23(25)15-14-22(24)26-17-19-12-13-20-10-7-8 |
| InchiKey: | QBKBHLPBVCMUNE-UHFFFAOYSA-N |
| Formula: | C23H30O4 |
| SMILES: | CCCCCCC(C)OC(=O)CCC(=O)OCc1ccc2ccccc2c1 |
| Mol. weight [g/mol]: | 370.48 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -118.07 | kJ/mol | Joback Method |
| hf | -596.80 | kJ/mol | Joback Method |
| hfus | 48.05 | kJ/mol | Joback Method |
| hvap | 89.29 | kJ/mol | Joback Method |
| log10ws | -7.02 | | Crippen Method |
| logp | 5.565 | | Crippen Method |
| mcvol | 306.590 | ml/mol | McGowan Method |
| pc | 1308.01 | kPa | Joback Method |
| rinpol | 2790.00 | | NIST Webbook |
| tb | 928.42 | K | Joback Method |
| tc | 1144.91 | K | Joback Method |
| tf | 549.93 | K | Joback Method |
| vc | 1.179 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 980.12 | J/molxK | 928.42 | Joback Method |
| cpg | 995.32 | J/molxK | 964.50 | Joback Method |
| cpg | 1009.37 | J/molxK | 1000.58 | Joback Method |
| cpg | 1022.31 | J/molxK | 1036.67 | Joback Method |
| cpg | 1034.21 | J/molxK | 1072.75 | Joback Method |
| cpg | 1045.12 | J/molxK | 1108.83 | Joback Method |
| cpg | 1055.12 | J/molxK | 1144.91 | Joback Method |
| dvisc | 0.0005856 | Paxs | 549.93 | Joback Method |
| dvisc | 0.0003381 | Paxs | 613.01 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002163 | Paxs | 676.09 | Joback Method |
| dvisc | 0.0001493 | Paxs | 739.17 | Joback Method |
| dvisc | 0.0001093 | Paxs | 802.26 | Joback Method |
| dvisc | 0.0000837 | Paxs | 865.34 | Joback Method |
| dvisc | 0.0000665 | Paxs | 928.42 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U370984&Units=SI |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/34-834-8/Succinic-acid-2-naphthylmethyl-2-octyl-ester.pdf>

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